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Deep geothermal resource assessment of the St. Lawrence Lowlands sedimentary basin (Québec) based on 3D regional geological modelling

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Abstract

Geothermal resource quantification requires underground temperature and volume information, which can be challenging to accurately assess at the regional scale. The analytical solution for steady-state heat conduction with internal heat generation is often used to calculate temperature at depth, while geological models can provide volume

information. Both approaches were originally combined in a single 3D geological model, in which the underground temperature is directly computed, to accurately evaluate geothermal resources suitable for power generation in the St. Lawrence Lowlands sedimentary basin covering 18,000 km² in Quebec, Canada, and improve methods for geothermal resource quantification. This approach, used for the first time at such a large scale, allowed to determine the volume of each thermal unit providing a detail assessment of resource depth, temperature and host geological formation. Only 5% of geothermal resources at a temperature above 120 °C that is suitable for power generation were shown to be hosted in the Cambro-Ordovician sedimentary rock sequences at a depth of 4 to 6 km, while 95% of the resource is hosted by the underlying Precambrian basement.

Keywords

Temperature; thermal; heat conduction; geothermal resource; enhance geothermal system.

Nomenclature

Symbols		Subscripts	
A	heat generation rate ($\mu\text{W m}^{-3}$)	e	effective or electrical
c	heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)	f	final
E	energy (J)	i	entity or initial
e	vertical thickness (m)	n	total number of entities
P	power (W)	PC	Precambrian basement
Q	heat flow (mW m^{-2})	r	rock
s	thermal diffusivity ($\text{m}^2 \text{sec}^{-1}$)	rec	recoverable
T	temperature ($^{\circ}\text{C}$)	sed	sedimentary
t	time (sec)	th	thermal
V	volume (m^3)	tot	total
$\Delta T/\Delta z$	geothermal gradient ($^{\circ}\text{C m}^{-1}$)	z	true vertical depths (TVD; m)
η	efficiency (%)	0	at the surface
λ	thermal conductivity ($\text{W m}^{-1} \text{K}^{-1}$)		
ρ	density (kg m^{-3})		
ϕ	proportion or recovery factor (%)		

1 Introduction

Three-dimensional (3D) modeling is nowadays widely used in regional to site scale geological projects. Geothermal resource assessments are following the trend and making use of different 3D models, both conceptual (e.g. Sausse *et al.*, 2010; Siler *et al.*, 2019) and numerical (e.g. Blöcher *et al.*, 2010; Zhao *et al.*, 2015), just to cite a few examples where models are used to better estimate geothermal system geometry, characteristics and geodynamics. 3D

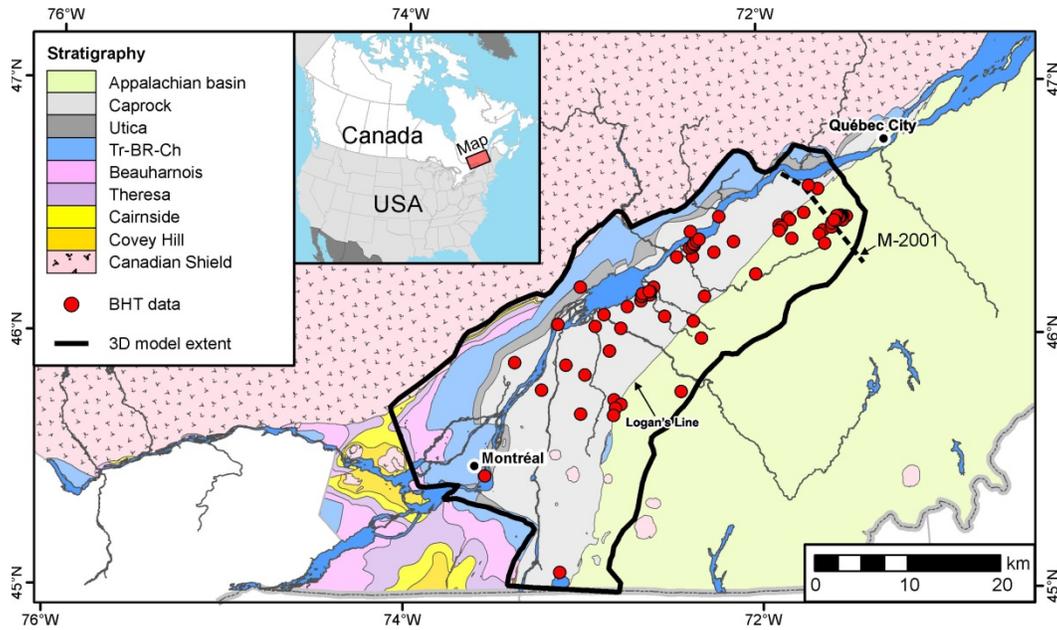
6 geophysical models based on inversion methods are also used for geothermal exploration and monitoring with
7 magnetotelluric, electrical resistivity, seismic and gravity data to better characterize the subsurface (Newman *et al.*,
8 2008; Nieto *et al.*, 2019).

9 Advances in 3D modeling software and computer capabilities are allowing to create large 3D geological models and
10 calculate temperature at depth based on heat transfer mechanisms. Moreover, as the geometry of the subsurface is
11 modelled in 3D, the volume and distribution of the geothermal targets can be evaluated more accurately, which is
12 one step forward in the assessment of the geothermal potential of a region. However, 3D geological models are not
13 commonly used for estimating geothermal resources at the regional or basin scale. Relatively small-scale 3D
14 geothermal models, on the order of ≤ 100 km in diameters, are described in the literature with non-exhaustive
15 examples from around the world including Denmark, Germany, Iceland, Italy, New Zealand, The Netherlands, the
16 United States of America and Taiwan (e.g. Guglielmetti *et al.*, 2013;; Chang *et al.*, 2014; Gasperikova *et al.*, 2015;
17 Ratouis *et al.*, 2016; Siler *et al.*, 2016; Przybycin *et al.*, 2017; Békési *et al.*, 2020; Fuchs, 2020). On the other hand,
18 regional or large-scale 3D models, on the order of >100 km diameters, are just starting to be used for the assessment
19 of geothermal resources. Recent examples of interest include the shallow geothermal potential assessment related to
20 ground source heat pumps by Santilano *et al.* (2016) in Italy and the basin-scale deep geothermal potential evaluation
21 for the French Massif Central by Calcagno *et al.* (2014), Central Alberta in Canada by Hofmann *et al.* (2014) and the
22 Williston Basin in the United States of America by Gosnold *et al.* (2016). How to properly develop such 3D regional
23 geological models and implement heat transfer equations to accurately evaluate temperature for estimating deep
24 geothermal resources remain challenging. Large-scale geothermal resource assessments tend to be conducted in 2D
25 (Blackwell *et al.*, 2006; Batir *et al.*, 2016; Stutz *et al.*, 2015; Palmer-Wilson *et al.*, 2018), where only surface heat
26 flow estimation is used to extrapolate temperature downward. In this study, an example of 3D geothermal resource
27 assessment for the St. Lawrence Lowlands (SLL) sedimentary basin in Québec, Canada, is provided using a
28 geological model covering an area of 230 by 75 km to address this challenge. The study illustrates how 3D
29 geological modeling can be originally combined with thermal characterization of stratigraphic units to extrapolate
30 temperature at depth using analytical solutions, considering the basin complex geometry, to properly estimate deep
31 geothermal resources. We believe this new 3D approach allows to better identify geothermal targets with appropriate
32 volume information compared to a conventional 2D approach.

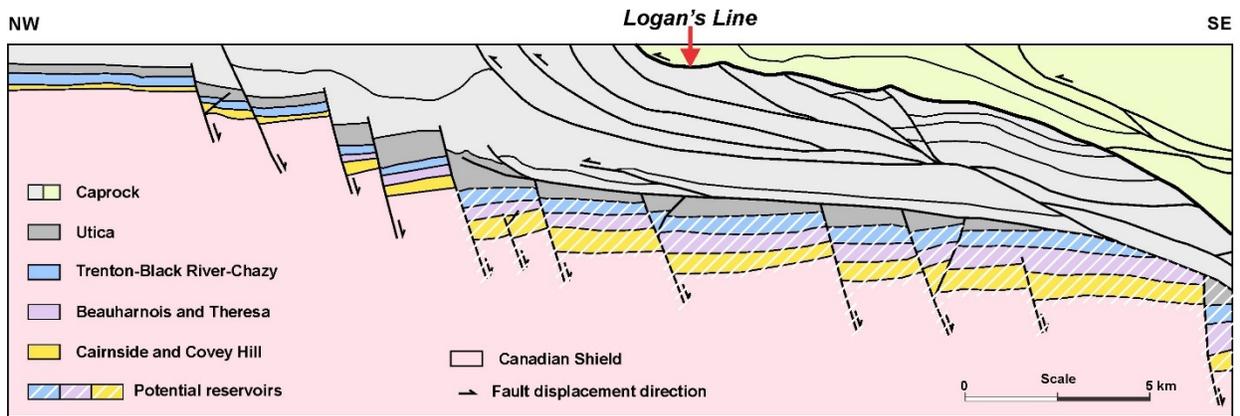
33 Previous geothermal studies of the SLL basin in southern Québec relied on raw and/or corrected bottom-hole
34 temperature (BHT) data obtained from oil and gas exploration wells combined with rock thermal conductivity
35 inferred from the literature (SNC-SOQUIP, 1979; e.g. Lefebvre et Trempe, 1980; Majorowicz et Minea, 2012;
36 Raymond *et al.*, 2012; Majorowicz et Minea, 2015b) to estimate temperature at depth. Recent works allowed to
37 present one-dimensional analysis of the geothermal state of the basin by defining thermal conductivity, heat
38 generation and temperature at depth evaluated by physical measurements of thermal properties of each stratigraphic
39 unit (Bédard *et al.*, 2017; Nasr *et al.*, 2018). The current manuscript follows previous work from Bédard *et al.* (2017)
40 in order to evaluate subsurface temperature in the 3D space as a further step, providing the missing volume
41 information to calculate the actual geothermal resource potential of the SLL basin. The new method developed in
42 this work allows obtaining accurate volume information to quantify and localize in the subsurface the thermal energy
43 content that can be converted to sustainable electricity. The original 3D geological model of the SLL basin (Bédard
44 *et al.*, 2013) was a key to determine this missing volume information, moving toward a first complete resource
45 quantification integrating in a novel fashion analytical heat transfer solutions in such a regional model. The use of a
46 large-scale 3D geological model as a support for heat transfer calculations to obtain a detailed estimate of the
47 temperature at depth is a significant advance for regional geothermal resource evaluation as it can be used to identify
48 energy content of specific geological formations with complex geometries, which can be difficult to achieve in 2D.

49 **2 Study area**

50 The study area of this project covers 18,000 km² in the southern part of the province of Québec, where most of the
51 population lives and hence has significant market potential for deep geothermal resources development. This region
52 also hosts parts of the strongest Canadian market for shallow geothermal installations (Canadian GeoExchange
53 Coalition, 2012). The area is actually located in the SLL sedimentary basin and partly in the Appalachian basin to the
54 south (Figure 1). The SLL basin unconformably overlies the Canadian Shield and is covered by the Appalachian
55 basin in the southeast. The SLL basin deepens toward the southeast because of the presence of NE-SW trending
56 normal faults as shown in Figure 2 (Konstantinovskaya *et al.*, 2009; Castonguay *et al.*, 2010). Most of the normal
57 faults only displaced the upper part of the Canadian Shield, also named the Precambrian basement, and the lower
58 part of the SLL sedimentary sequence as shown in Figure 2.



59
 60 **Figure 1. Geological map of southern Québec province showing the thermal units, the extent of the 3D model**
 61 **and BHT data used in this study. The black dashed line shows the location of M-2001 seismic line (Figure 2).**



62
 63 **Figure 2. SLL sedimentary basin architecture and thermal units based on M-2001 seismic line with ~2X**
 64 **vertical exaggeration. Modified from Castonguay *et al.* (2010). See Figure 1 for location.**

65 This manuscript uses the concept of thermal units that are defined as consecutive geological layers of similar thermal
 66 conductivity and heat generation rate. Considering that thermal properties of rocks are strongly linked to their
 67 physical properties, the SLL basin is divided in seven thermal units (Bédard *et al.*, 2017; Raymond *et al.*, 2017)
 68 based on the standard lithostratigraphy of the SLL basin proposed by Comeau *et al.* (2013), with one more thermal
 69 unit used to represent the Canadian Shield or the Precambrian basement (Figure 1; Figure 2; Table 1).

70 The Caprock thermal unit is composed of the Queenston, Lorraine and Sainte-Rosalie groups as well as the rocks
 71 from the Appalachian basin. The Cambro-Ordovician Appalachian basin is composed of various deformed

72 sedimentary rocks that are not differentiated in the 3D model used in this study. The sedimentary rocks of the
73 Caprock unit are composed of fine-grained siliciclastics, carbonates and shales acting as caprocks with low
74 permeability and potential thermal blanket with relatively low thermal conductivity (Table 1). Underlying carbonate
75 rocks of the Trenton-Black River-Chazy (Tr-BR-Ch) unit are grouped in a single thermal unit in the 3D model
76 because their physical and thus thermal characteristics are similar. The Beauharnois and Theresa units are composed
77 of dolostones grading to dolomitic sandstones and show higher thermal conductivity, with a low matrix porosity on
78 the order of 1~2 % (Tran Ngoc *et al.*, 2014). However, the secondary porosity of the Beauharnois and Theresa units
79 can reach up to 15 % in dolomitic facies due to dissolution along fractures (Bertrand *et al.*, 2003). The clastic rocks
80 of the Cairnside and Covey Hill thermal units show the highest thermal conductivity due to their important quartz
81 content (Table 1). The Canadian Shield is made up of Precambrian igneous, volcanic and metamorphic rocks that are
82 not differentiated in the 3D model and are thus considered as a uniform thermal unit (PC) in this study. With their
83 position at the base of the sedimentary sequence where temperature is higher and because of their potentially higher
84 permeability, the Covey Hill and Cairnside thermal units as well as the fractured basement rocks just below the basin
85 are the principal targets for hydrothermal resources in the SLL basin. The Covey Hill and Cairnside units have a
86 porosity between 4 to 6 % and values that can locally exceed 10 % (Tran Ngoc *et al.*, 2014). Enhanced geothermal
87 systems (EGS) is further considered for the Canadian Shield deep below the basin (Majorowicz and Minea, 2015a).

88 The input parameters presented in Table 1 were used to estimate the 3D subsurface temperatures of the SLL basin in
89 this study and are described with more detail in Bédard *et al.* (2017). This previous study defined the thermal
90 conductivity and heat generation rate of the different thermal units based on rock sample measurements conducted in
91 the laboratory and on well log analysis (Nasr *et al.*, 2015; 2018). The basement PC unit was sampled North of the
92 basin where the unit crops out and in rare boreholes that reached this unit in order to define thermal properties below
93 the basin and extrapolate temperature at depth. The input temperature data were corrected for both drilling
94 disturbance and paleoclimatic variations in order to estimate the surface heat flow associated with BHT locations
95 (Bedard *et al.*, 2014). It is important to note that deep geothermal resources exploration in the SLL is at an early
96 stage and, as a consequence, there is no equilibrium temperature data available below ~300 m depth. The 81 BHT
97 data used in this study were recorded at a depth varying from 660 to 4,329 m (Figure 1). The estimated equilibrium
98 geothermal gradient taking into account the above corrections ranges from 12.2 to 40.4 °C, with an average of $24.3 \pm$
99 $4.9 \text{ }^\circ\text{C km}^{-1}$ (Bédard *et al.*, 2017). Temperature predictions below the deepest borehole, made with the methodology

100 described below, mostly relied on the surface outcrops of the analysed PC unit used as analogues of the deep
 101 subsurface.

102 **Table 1. Characteristics of the SLL basin thermal units. Caprock data include the Sainte-Rosalie, Lorraine**
 103 **and Queenston groups as well as the Appalachian basin. Tr-BR-Ch: Trenton-Black River-Chazy unit.**

Age	Thermal unit	Lithology	Thermal conductivity ^a (W m ⁻¹ K ⁻¹)	Heat generation rate ^a (μW m ⁻³)	Heat capacity ^b (J kg ⁻¹ K ⁻¹)	Rock density ^{a,b} (kg m ⁻³)					
ORDOVICIAN	U	Caprock	<i>Shales</i> <i>Siltstones</i> <i>Sandstones</i> <i>Limestones</i>	2.79 ± 0.75	1.59 ± 0.28	890	2,700				
		Utica						2.52 ± 0.31	0.95 ± 0.37	832	2,450
		Tr-BR-Ch						2.85 ± 0.46	0.41 ± 0.27	852	2,700
	M	Beauharnois						3.80 ± 0.62	0.69 ± 0.27	862	2,740
	L	Theresa						4.29 ± 1.44	0.94 ± 0.30	847	2,705
CAMBRIAN	U	Cairnside	6.19 ± 0.60	0.25 ± 0.14	827	2,650					
		Covey Hill	4.78 ± 1.22	0.79 ± 0.28	796	2,630					
	M										
PC	Canadian Shield	<i>Igneous,</i> <i>volcanic and</i> <i>metamorphic</i>	3.00 ± 0.78	N/A	762	2,598					

104 ^a Data source: Bédard *et al.* (2017) and references therein. ^b Data source: Nasr *et al.* (2015); Nasr (2016).

105 **3 Methodology**

106 This study aims at estimating the 3D subsurface temperature of the SLL basin and the underlying basement, up to
107 13 km, with the use of a 3D geological model in which thermal properties are distributed respecting the 3D geometry
108 of the thermal units at depth. The basin deep temperature is then used to assess the geothermal resource base
109 according to the methodology used by MIT (2006). Both resources associated to the basement with potential for EGS
110 technologies and associated to the basal sedimentary units that can host natural reservoirs are considered although
111 most of the resource that can be used for power generation is located in the basement.

112 **3.1 Temperature at depth**

113 The 3D geological model of the SLL basin, previously constructed with the GOCAD software and presented by
114 Bédard *et al.* (2013), was used as the basis for the 3D temperature assessment of the basin. In the model, the
115 geological map of the area defines the location of rock units at surface and was combined with a structural map of
116 the Precambrian basement top in two-way travel time units converted to depth with well data to further constrain the
117 geometry and depth of the Precambrian basement. Geophysical well logs from 81 oil and gas exploration wells were
118 reinterpreted and used to determine the elevation of rock unit contacts to provide an extensive dataset with a total of
119 441 contact locations and built the 3D geological model. The location of major faults was defined according to the
120 map of the Precambrian basement depth and differences in elevation between the rock unit contacts in wells. Some
121 modifications to the initial model were achieved to comply with the geothermal assessment objective. The original
122 model was extended toward the southeast to include more data and take possible temperature anomalies into account.
123 The 3D model was also extended to a depth of 13 km, which meant to extend the PC thermal unit downward. Each
124 3D cell of the model has a distinct thermal conductivity, heat generation rate, thermal capacity and rock density that
125 are defined according to the thermal unit in which the cell belongs. This allows having a more realistic distribution of
126 the parameters in the 3D space as a function of the thermal unit depth and thickness that vary in the basin. This study
127 assumes a purely vertical conductive heat transfer in the basin. The analytical solution for steady-state heat
128 conduction with internal heat generation was actually implemented in the GOCAD software to evaluate temperature
129 at depth. Moreover, because of the lack of sufficient data to estimate spatial distributions of the parameters, thermal
130 conductivity and heat generation rates are both defined as homogeneous in each thermal unit and then, do not vary
131 with depth, temperature or location.

132 Effective thermal conductivity and heat generation rate are calculated assuming that heat flow is vertical. The
 133 effective thermal conductivity λ_e is calculated cell by cell directly in the 3D model with a harmonic mean of the
 134 thermal conductivity from the surface downward following the equation:

$$135 \quad \frac{1}{\lambda_e} = \sum_{i=1}^n \frac{\phi_i}{\lambda_i} \quad (1)$$

136 where λ_i ($\text{W m}^{-1} \text{K}^{-1}$) is the thermal conductivity of the i -cell and ϕ_i (%) is the thickness proportion of the i -cell
 137 compared to the total thickness from the n -cell to the surface.

138 The effective heat generation rate A_e is calculated cell by cell in the 3D model with a weighted arithmetic mean of
 139 the heat generation rate from the surface downward following the equation:

$$140 \quad A_e = \frac{\sum_{i=1}^n (A_i \cdot e_i)}{\sum_{i=1}^n e_i} \quad (2)$$

141 where e_i (m) is the thickness of the i -cell with the given heat generation rate A_i (W m^{-3}).

142 The distribution of the surface heat flow has been interpolated for the entire SSL basin using 81 surface heat flow
 143 values $Q_{0,P50}$ calculated from deep corrected BHTs (Bédard *et al.*, 2017). Simple kriging (SK) was used to spatialize
 144 the Q_0 values over the entire area of the model. This method is well known for interpolating sparse continuous
 145 properties, while considering spatial correlation (Srivastava, 1994). The experimental variogram was calculated on
 146 raw data and the variogram was best modelled by a spherical function with a range of 40 km, a sill of 1 and a nugget
 147 effect of 40%.

148 The temperature of sedimentary rock units is calculated cell by cell directly in the 3D geological model from the
 149 surface downward by using the linear decrease relationship theory that characterizes the internal heat generation,
 150 with the following equation implemented in GOCAD (e.g. Jessop, 1990; Stein, 1995; Turcotte and Schubert, 2014):

$$151 \quad T_{z(\text{sed})} = T_0 + \left(\frac{Q_0 \cdot z_{\text{sed}}}{\lambda_{e,z}} \right) - \left(\frac{A_{e,z} \cdot z_{\text{sed}}^2}{2\lambda_{e,z}} \right) \quad (3)$$

152 where $T_{z(\text{sed})}$ ($^{\circ}\text{C}$) is the temperature at depth z in the sedimentary rocks; T_0 is the average surface temperature (8°C);
 153 Q_0 (W m^{-2}) is the surface heat flow; z_{sed} (m) is the depth in the sedimentary rocks; $\lambda_{e,z}$ ($\text{W m}^{-1} \text{K}^{-1}$) is the effective
 154 thermal conductivity at depth z ; and $A_{e,z}$ (W m^{-3}) is the average heat generation rate at depth z .

155 The exponential decrease relationship theory, developed by Lachenbruch (1970), is used in this study to extrapolate
156 temperature at depth of the Canadian Shield thermal unit cell by cell from the top to bottom, using the following
157 equation in GOCAD (e.g. Jessop, 1990; Turcotte and Schubert, 2014):

$$158 \quad T_{z(PC)} = T_{PC} + \left(\frac{Q_{PC} \cdot z_{PC}}{\lambda_{PC}} \right) - \left(\frac{A_{PC} \cdot e_{PC}^2 \cdot \left[1 - \exp\left(-\frac{z_{PC}}{e_{PC}}\right) \right]}{\lambda_{PC}} \right) \quad (4)$$

159 where $T_{z(PC)}$ (°C) is the temperature at depth in the Precambrian; T_{PC} (°C) is the temperature at the top of the
160 Precambrian; Q_{PC} (W m⁻²) is the calculated heat flow at the top of the Precambrian; z_{PC} (m) is the depth from the top
161 of the Precambrian; λ_{PC} (W m⁻¹ K⁻¹) is the thermal conductivity of the Precambrian; A_{PC} (W m⁻³) is the heat
162 generation rate of the Precambrian; and e_{PC} (m) is the total thickness of the Precambrian considered in the 3D model.
163 The use of the two different equations to calculate the temperature in the sedimentary succession and in the
164 Precambrian basement is still debated in the scientific community and can difficultly be confirmed (Turcotte and
165 Schubert, 2014). Equation (2) was used to take into account the heat generation of the radiogenic elements assumed
166 to be uniform in each sedimentary rock unit (Equation 3) and to decrease exponentially in the igneous and
167 metamorphic rocks of the basement (Equation 4). This approach to calculate temperature at depth takes into account
168 the different nature of the sedimentary versus crystalline rock of the basement. The base of the 3D model is set to
169 13 km to perform the downward temperature extrapolation taking into account the thickness of the sedimentary
170 sequence as proposed by Blackwell *et al.* (2006). The calculation of A_{PC} and e_{PC} developed in Bédard *et al.* (2017)
171 are used in this paper in order to get the values of those parameters. It must be noted that heat generation rate of the
172 Precambrian A_{PC} is assumed to be constant at depth for each location. Consequently, this approach results in an
173 adjustment of the heat generation rate of the Precambrian A_{PC} for each location based on the corrected input
174 temperature data and assuming a constant mantle heat flow of 15 W m⁻² (Bédard *et al.*, 2017). Therefore, thermal
175 anomalies recorded in oil and gas exploration wells are assumed to be caused by variations of concentration of
176 radiogenic elements in the underlying Precambrian thermal unit. Input temperature data used at this point have been
177 previously corrected for paleoclimate variation to estimate heat flow further used to extrapolate the theoretical
178 undisturbed temperature in the absence of paleoclimate perturbations. The paleoclimate correction is thus removed as
179 a last step from the calculation of extrapolated temperature in order to obtain an estimate of the actual subsurface
180 temperature.

181 3.2 Geothermal resources

182 The subsurface temperature being assessed, the estimation of the geothermal resources was then achieved with the
183 3D model calculating the thermal energy in place or heat volume (i.e. MIT, 2006; Williams *et al.*, 2008). The use of
184 the 3D model allows to directly calculate an accurate volume of each thermal unit with geothermal potential at depth
185 based on the exact basin geometry that is fairly complex. In the case of the SLL, calculations have been achieved on
186 1 km thick layers from 3 to 10 km depth for temperature ranges of 120 to 150 °C and more than 150 °C. Moreover,
187 the use of the 3D model allowed estimating the resources for three different geological entities: 1) all the potential
188 reservoir units of the sedimentary sequence from the Tr-BR-Ch to the Covey Hill thermal units; 2) the Cairnside and
189 Covey Hill only; and 3) the Canadian Shield (PC unit). The assessment of the total geothermal energy content E_{tot} (J)
190 is calculated with:

$$191 E_{\text{tot}} = \rho \cdot c \cdot V_r \cdot (T_i - T_0) \quad (5)$$

192 where ρ (kg m⁻³) is the rock density; c (J kg⁻¹ °C⁻¹) is the heat capacity; V_r (m³) is the rock volume; T_i (°C) is the
193 initial rock temperature; and T_0 (8°C) is the average surface temperature.

194 Following the method used by MIT (2006), the recoverable energy is constrained by a recovery factor that was set to
195 2 and 20 % (pessimistic and optimistic heat recovery scenarios), as well as by the reservoir temperature drop that is
196 limited to 10 °C in order to keep sustainable reservoir conditions during system operation. The recoverable energy
197 was thus calculated with:

$$198 E_{\text{rec}} = E_{\text{tot}} \cdot \frac{(T_i - T_f)}{(T_i - T_0)} \cdot \phi \quad (6)$$

199 where E_{rec} (J) is the recoverable geothermal energy; E_{tot} (J) is the total geothermal energy content; T_i (°C) is the
200 initial rock temperature; T_f (°C) is the final rock temperature; $T_i - T_f$ (10 °C) is the maximum reservoir temperature
201 drop; T_0 (8 °C) is the average surface temperature; and ϕ (%) is the recovery factor.

202 Once the recoverable geothermal energy is determined, it is finally converted in useful energy, which is electricity in
203 this case, where it is estimated in the context of a binary power plant with an operation period of 30 years. The
204 recoverable electric power is calculated following:

$$205 P_e = \frac{E_{\text{rec}} \cdot \eta_{\text{th}}}{t} \quad (7)$$

206 where P_e ($J s^{-1}$ or W) is the electrical power; E_{rec} (J) is the recoverable geothermal energy; η_{th} (%) is the
207 thermodynamic efficiency and t (sec) is the exploitation lifetime. For typical binary power plant, in which the
208 geothermal fluid temperature is between 100 and 165 °C (MIT, 2006), the net thermodynamic efficiency is:

$$209 \quad \eta_{th} = (0,0935 \cdot T_i) - 2,3266 \quad (8)$$

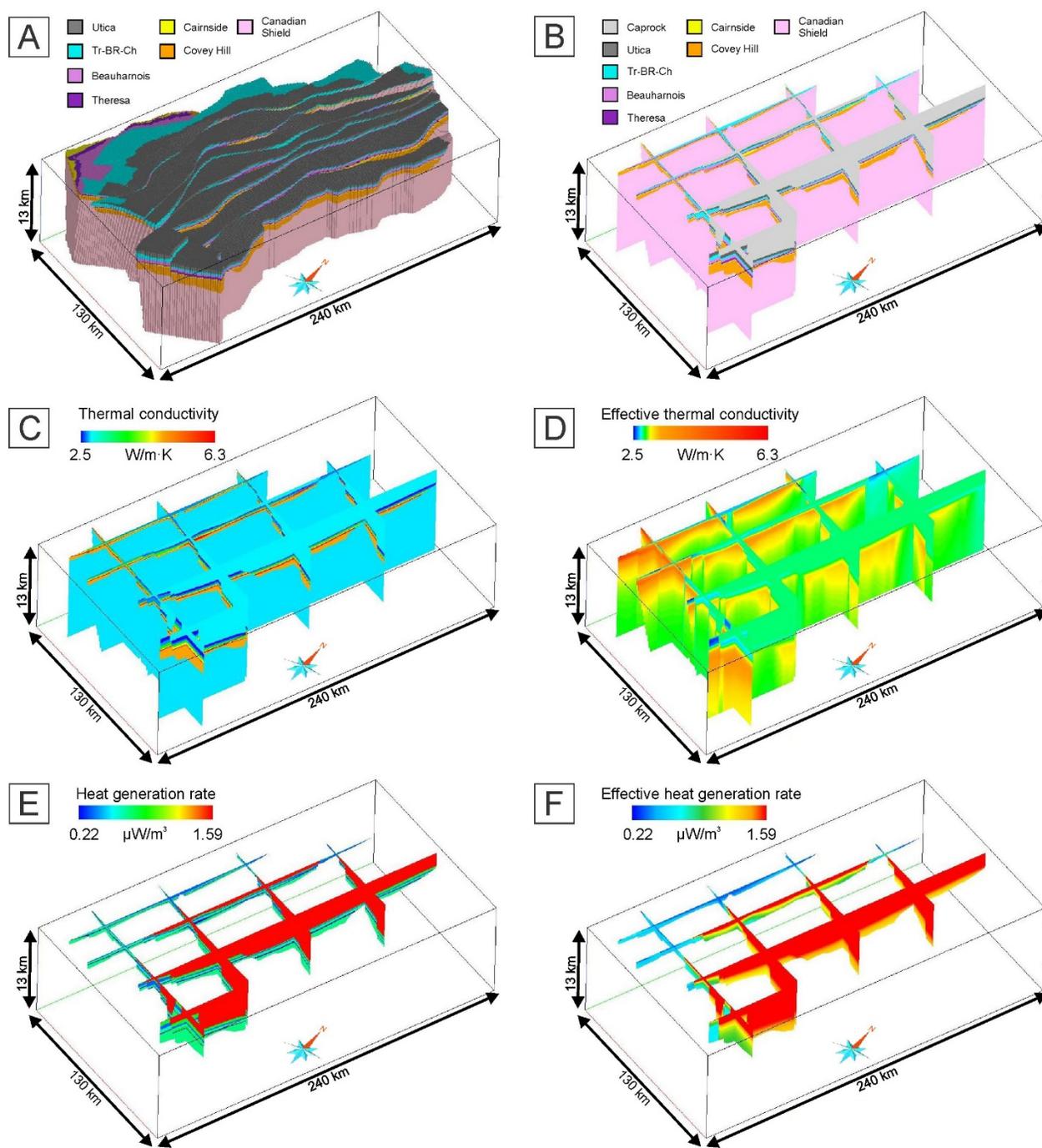
210 where η_{th} (%) is the thermodynamic efficiency and T_i is the initial rock temperature (°C).

211 **4 Results**

212 **4.1 Temperature at depth**

213 The size of the SLL basin 3D model used in this study is 240 x 130 km by 13 km thick with cells of 753 x 1,004 m
214 by 10 m thickness. The long axis of the model is oriented SW-NE to comply with the anisotropic geometry of the
215 basin. The 3D model includes 30,239,173 cells that are grouped in eight thermal units (Figure 3A and B).

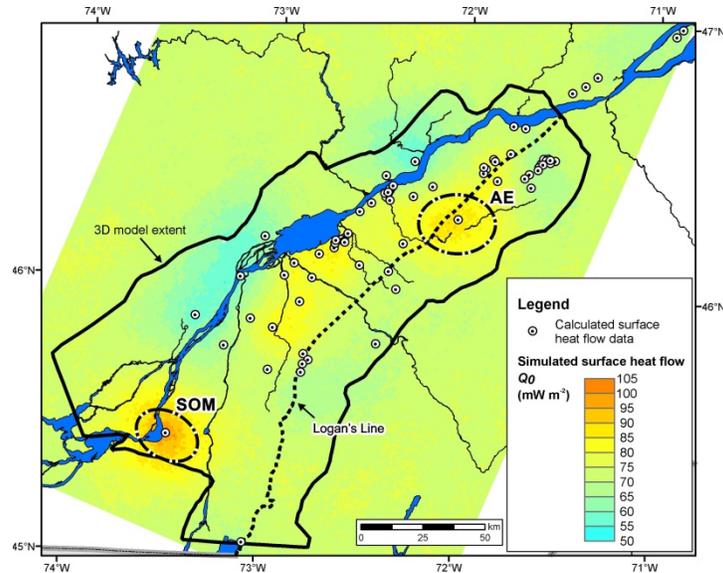
216 As shown in Figure 3C and E, both the thermal conductivity and the heat generation rate are constant in each of the
217 eight thermal units. The use of the 3D model allows calculating the effective thermal conductivity and heat
218 generation rate at depth taking into account the 3D geometry of the units at the basin scale (Figure 3D and F).



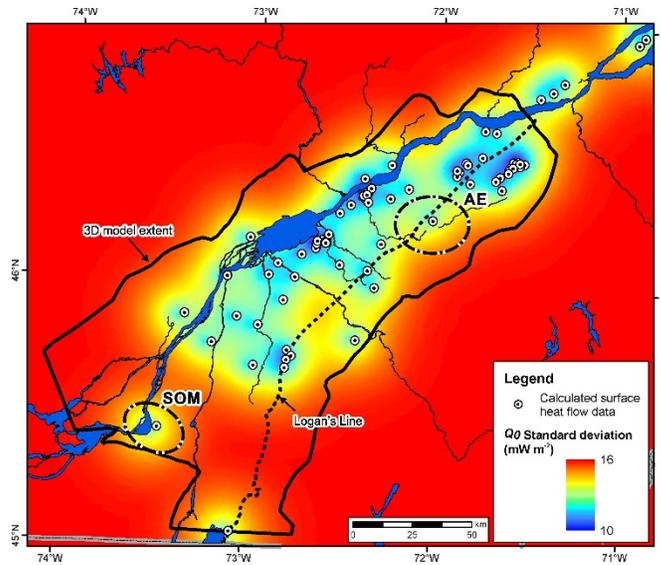
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221 **Figure 3. 3D geological model of the SLL basin with thermal units and their properties. (A) Volume model**
 222 **without the Caprock thermal unit. Vertical cross-sections showing (B) the architecture of the 3D model, the**
 223 **3D distribution of (C) the thermal conductivity, (D) the effective thermal conductivity, (E) the heat generation**
 224 **rate for the sedimentary sequence and (F) the effective heat generation rate for the sedimentary sequence.**
 225 **Vertical exaggeration: 5X.**

226 The surface heat flow is mapped with kriging in Figure 4 and its associated standard deviation is shown in Figure 5.
 227 The kriging map of the heat flow highlights 2 positive heat flow anomalies aligned North-South along the south
 228 shore of St. Lawrence river and a low trend along north shore. The main goal here was not to obtain an accurate
 229 surface heat flow map from equilibrium temperature data since appropriate equilibrium temperature profiles for deep
 230 wells are not available in the SLL basin such that basin scale heat flow can only be estimated from BHT data.
 231 Important uncertainty consequently remains about heat flow distribution in the basin. Accordingly, this surface heat
 232 flow map can be seen as an intermediate step in the methodology to compute the 3D temperature distribution at
 233 depth. It is strictly dependent on the input BHT data, but this does not affect the 3D approach presented in this
 234 manuscript. Geothermal exploration in the SLL basin is at an early stage and equilibrium temperature data can be
 235 integrated as it will become available when geothermal exploration moves to further steps. Thereby, the heat flow
 236 assessment can difficultly be compared to previous and actual heat flow maps of the study area, which rely on
 237 shallow wells with equilibrium temperature data and commonly tend to display lower values of heat flow for the
 238 region (e.g. Saull *et al.*, 1962; Mareschal *et al.*, 1989; Guillou-Frottier *et al.*, 1995; Blackwell et Richards, 2004;
 239 Majorowicz et Minea, 2012).



240
 241 **Figure 4. Distribution of surface heat flow of the SLL basin generated by kriging surface heat flow estimated**
 242 **at oil and gas exploration wells. Black ellipses show the positive anomalies of the surface heat flow. SOM:**
 243 ***Southeast of Montreal anomaly. AE: Arthabaska-Érable anomaly.***



244

245

Figure 5. Standard deviation associated to surface heat flow kriging.

246

The 3D subsurface temperature distribution is calculated from previously defined parameters until the base of the

247

sedimentary sequence. The temperature at the base of the sedimentary sequence is then used to evaluate the heat

248

generation rate of the Precambrian A_{PC} (Figure 6). The anomalies in the heat generation rate of the Precambrian

249

thermal unit are related to the surface heat flow anomalies shown in Figure 4. It is therefore assumed that anomalies

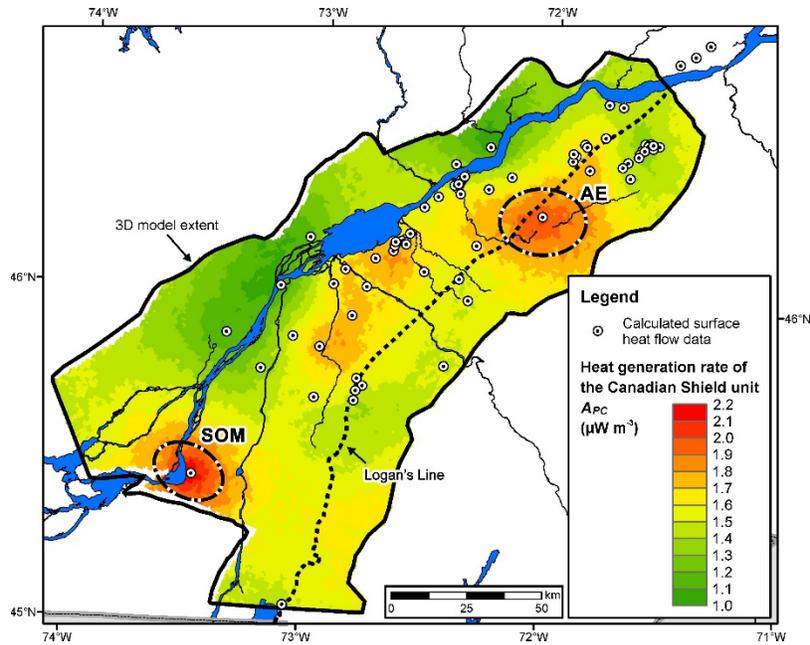
250

in heat generation rate and surface heat flow are caused by varying concentration of radiogenic elements in the

251

underlying Canadian Shield (PC unit).

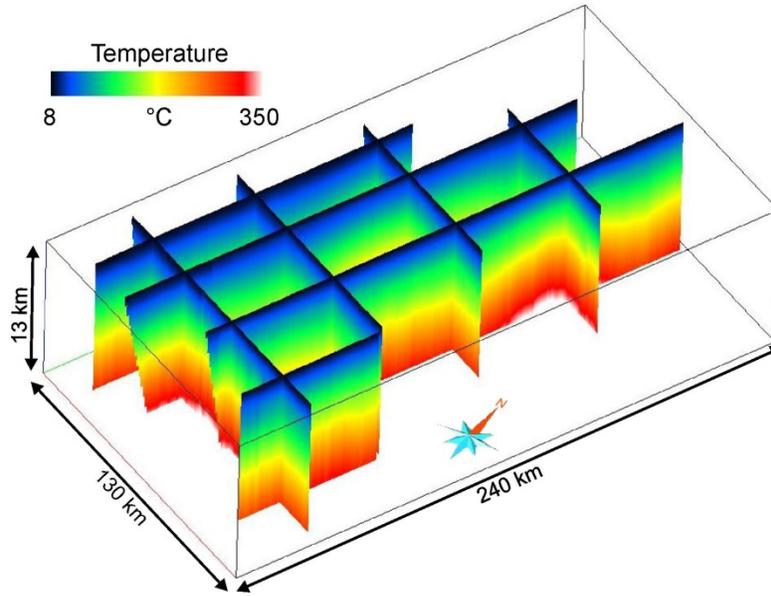
252



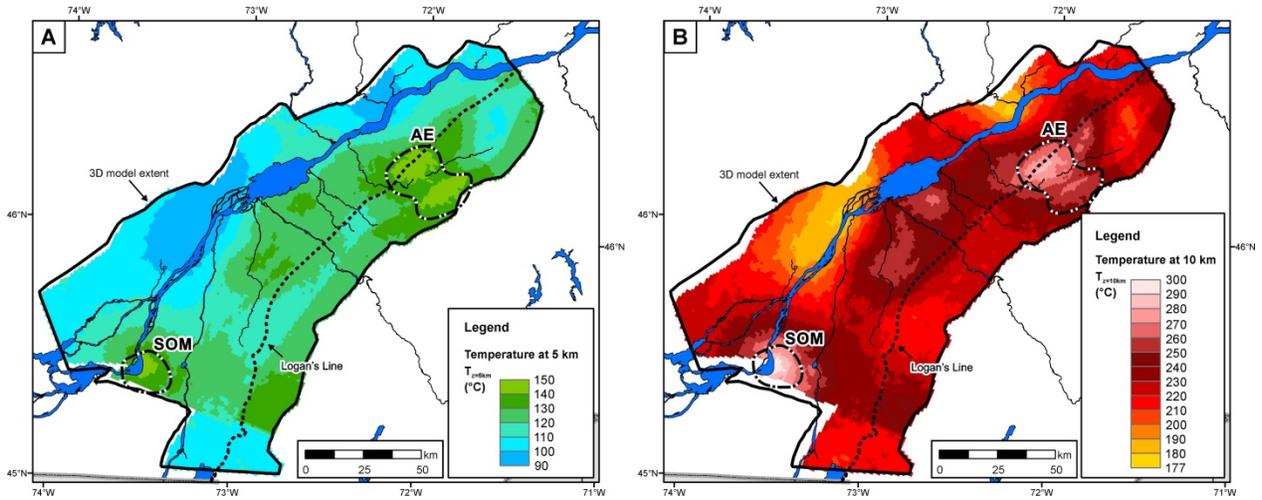
253

254 **Figure 6. Distribution of heat generation rate calculated for the Canadian Shield thermal unit. Black ellipses**
 255 **show the positive anomalies of the surface heat flow. SOM: Southeast of Montreal anomaly. AE: Arthabaska-**
 256 **Érable anomaly.**

257 Finally, the temperature in the Precambrian basement is calculated and merged with the sedimentary sequence
 258 temperature while reprocessing for the paleoclimate correction in order to provide a complete 3D subsurface
 259 temperature model of the SLL at present time (Figure 7). The calculated temperature varies from 8 °C at the surface
 260 to 150 °C at 5 km depth and 300 °C at 10 km depth in the anomalies of *Southeast of Montreal* (SOM) and
 261 *Arthabaska-Érable* (AE; Figure 8). The SOM anomaly is constrained by one BHT data point only while wells
 262 surrounding the AE anomaly suggest a stronger heat flow that peaks toward the well with higher BHT.



263
 264 **Figure 7. Cross-sections view of the calculated subsurface temperature in the SLL basin and the underlying**
 265 **Canadian Shield.**

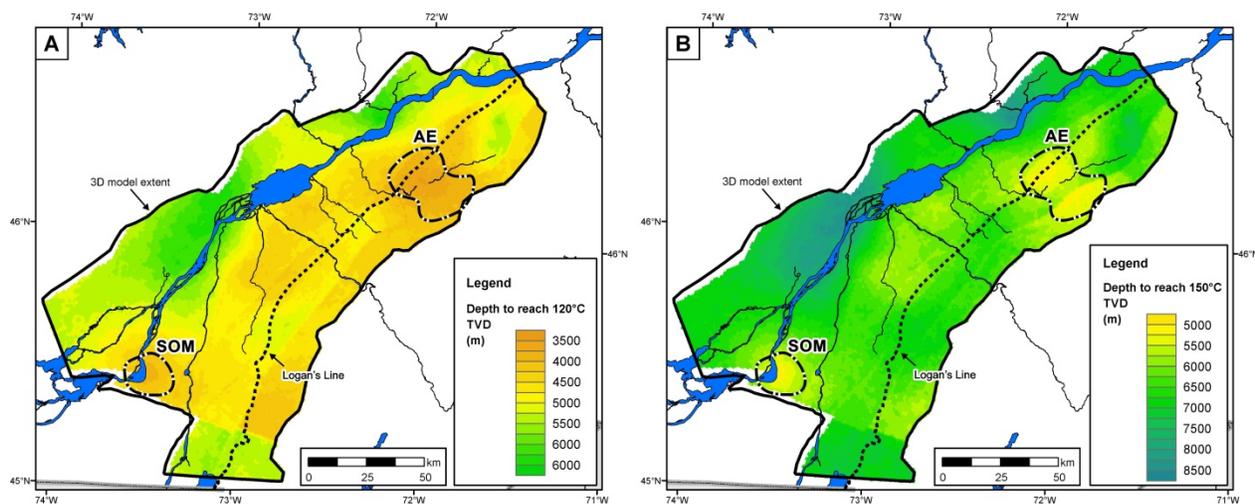


266
 267 **Figure 8. Calculated subsurface temperature at A) 5 km depth and B) 10 km depth. SOM: *Southeast of***
 268 ***Montreal anomaly. AE: Arthabaska-Érable anomaly.***

269 **4.2 Geothermal resources**

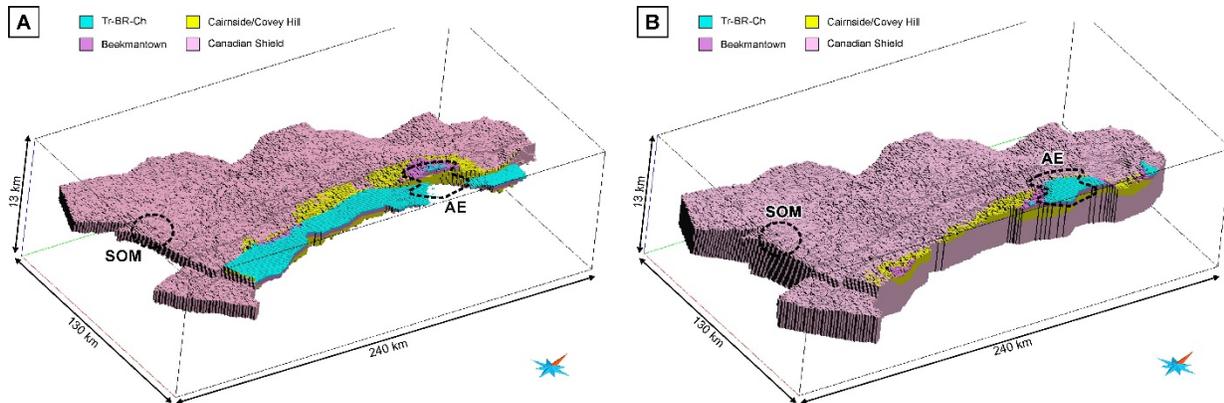
270 The use of the 3D model allowed to compute the total amount of thermal energy that can be recovered from each
 271 unit, some sedimentary units having reservoir potential while the Precambrian basement is mostly associated to EGS.
 272 Threshold temperatures of 120 and 150 °C have been used to assess geothermal resources for power generation. The
 273 depth at which 120 °C is found is between 3,700 and 6,800 m, with an average of 5,200 m, while the shallower depth
 274 is located to the AE anomaly (Figure 9A). A temperature of 150 °C is reached between 5,000 and 8,500 m depth,

275 with an average of 6,500 m and the shallowest depth in the AE and SOM anomalies (Figure 9B). The units with
276 geothermal potential having temperature between 120 and 150 °C are thus located between 3 and 9 km depth (Figure
277 10A) and reach a maximum thickness of 2,000 m. Units with temperature higher than 150 °C are found between 5
278 and 10 km depth (Figure 10B). The SSL sedimentary basin thickness at the location of the SOM temperature
279 anomaly is less than 1,800 m such that a temperature greater than 120 °C is found in the Canadian Shield thermal
280 unit only. Temperature above 120 °C in the AE anomaly is found both in the SSL thermal units with potential
281 reservoir characteristics and in the Precambrian thermal unit. The SSL basin in the northern part of the AE anomaly
282 is in the 120-150 °C temperature range with an average thickness of 925 m (975 m for the combined Cairnside and
283 Covey Hill thermal units) while the SSL basin above 150 °C has an average thickness of 1,170 m (700 m for the
284 combined Cairnside and Covey Hill thermal units) in the southern part of the anomaly.



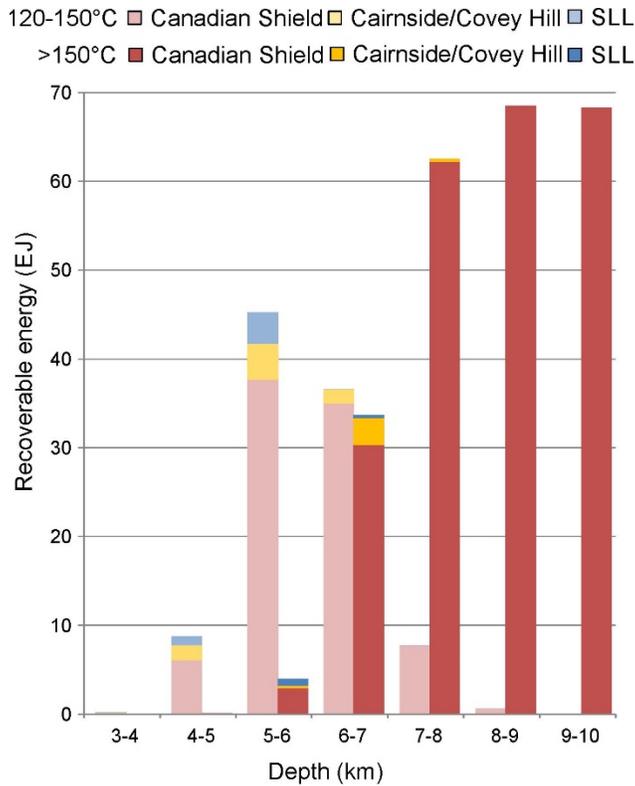
285
286 **Figure 9. A) Depth to reach 120 °C. B) Depth to reach 150 °C. SOM: Southeast of Montreal anomaly. AE:**
287 **Arthabaska-Érable anomaly. TVD: True Vertical Depth.**

288

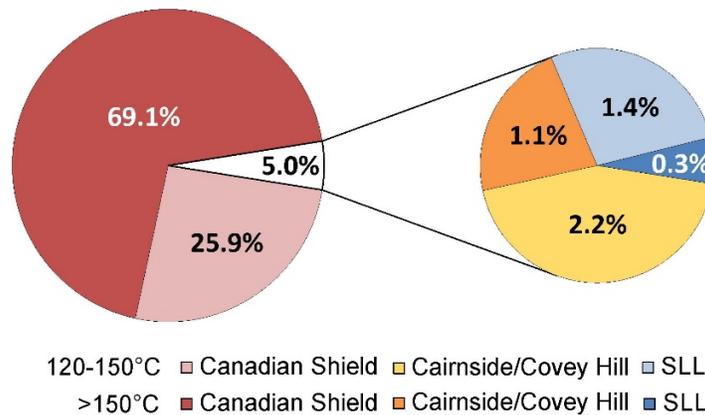


289
 290 **Figure 10. 3D geological model showing thermal units A) between 120 and 150 °C and B) above 150 °C and**
 291 **down to 10 km depth. SOM: *Southeast of Montreal* anomaly. AE: *Arthabaska-Érable* anomaly.**

292 The total geothermal energy (eq. 5) present in all thermal units, including the Canadian Shield, with temperatures
 293 above 120 °C and down to 10 km is in the order of 25,000 EJ. The total recoverable geothermal energy (eq. 6) of the
 294 SSL basin is in the order of 320 EJ and 32 EJ, when considering recovery factors of 20% and 2%, respectively
 295 (Figure 11). About 95 % of this energy is contained in the Canadian Shield (PC unit), which also represents the most
 296 important volume among all thermal units between 3 and 10 km depth (Figure 12). The geothermal energy present in
 297 the SSL basin is mostly available between 4 and 7 km depth at temperatures between 120 and 150 °C. The
 298 geothermal energy contained in the combined Cairnside and Covey Hill thermal units with potential reservoir
 299 characteristics contains the greater proportion of the energy among the sedimentary rock units. Geothermal resources
 300 with temperature above 150 °C in the combined Cairnside and Covey Hill thermal units is mainly available between
 301 6 and 7 km depth and is on the order of 3 and 0.3 EJ when considering a 20% and 2% recovery factor, respectively.



302
 303 **Figure 11. Recoverable energy considering a 20% recovery factor for the thermal units above 120 °C. SSL:**
 304 **sedimentary units with potential reservoir characteristics without the Cairnside and Covey Hill thermal units.**



305
 306 **Figure 12. Distribution of the recoverable geothermal energy down to 10 km depth in the different thermal**
 307 **units. SSL: sedimentary units with potential reservoir characteristics without the Cairnside and Covey Hill**
 308 **thermal unit.**

309 The electrical power estimated in the context of a binary power plant with 30 years exploitation period is on the
 310 order of 45,000 MWe for all the thermal units with potential reservoir characteristics and the basement above
 311 120 °C, when considering a recovery factor of 20%. This is similar to the total electrical power actually installed in
 312 the Province of Québec (Table 2). The electrical power estimated with a 2% recovery factor is consequently

313 4500 MWe, which is similar to the hydroelectric power plant of Churchill Falls (Table 2). More precisely, the
314 electrical power associated with the combined Cairnside and Covey Hill thermal unit above 150 °C is mainly
315 available between 6 and 7 km depth and is on the order of 400 and 40 MWe, considering a recovery factor of 20%
316 and 2%, respectively.

317 **Table 2. Power generation in the Province of Québec (Hydro-Québec, 2017).**

Power plant capacity at the end of 2017	MW
Hydroelectric power plants (70)	36,874
Churchill Falls power plant (Labrador)	5,428
Wind farms (39)	3,508
Thermal plants (24)	542
Biomass and biogas cogeneration plants (12)	272
Others	988
Total	47,612

318

319 **5 Discussion and conclusions**

320 The 3D temperature model presented in this paper was used to accurately assess geothermal resources of thermal
321 units in the SLL, including the underlying Canadian Shield and considering the sedimentary basin architecture. The
322 volume estimate was based on the number of 3D cells having the appropriate threshold temperatures of 120 °C and
323 150 °C, allowing to calculate the geothermal energy available in the SSL basin as function of temperature, depth and
324 thermal unit distribution. Evaluation of energy content in each thermal unit as shown in Figure 11 is a new
325 information for the SLL basin that could not have been obtained with previous 1D or 2D modeling approaches
326 (Majorowicz and Minea, 2012; Bédard *et al.*, 2017). The 3D geological model, incorporating analytical heat transfer
327 solutions, is a powerful tool to rapidly compute geothermal resources and illustrate which thermal units contains the
328 energy, at what depth and where. In the 3D model, only 5 % of the total geothermal resource that is appropriate for
329 power generation (25,000 EJ) is located in the SSL basin units with potential reservoir characteristics at depth greater
330 than 4 km. Consequently, the vast majority of the geothermal resources for power generation is located in the
331 Canadian Shied, which is not considered as a conventional reservoir rock and, therefore, implies the use of EGS.
332 Reservoir stimulation appears a key to unlock deep geothermal resources of the SLL basin. This shows the added
333 value of a geothermal resource estimated based on a 3D geological model, offering more information on resource

334 location, a significant advance compared to previous 1D and 2D geothermal resources assessments (Majorowicz and
335 Minea, 2012; Bédard *et al.*, 2017).

336 The use of a 3D regional geological model, in which steady-state conductive heat transfer equations have been
337 implemented, brings resource quantification to a high level and was proven valuable to identify regional targets with
338 geothermal resources at shallower depth. The evaluation of temperature distribution revealed two anomalies with a
339 higher temperature at shallower depth, when compared to the basin average temperature distribution, and therefore
340 greater geothermal potential. As the Cairnside and Covey Hill thermal units show the higher porosity of the
341 sedimentary sequence, they represent, together with the potentially fractured basement at the basin interface, the
342 most suitable target for geothermal exploration. The AE anomaly appears to be the area of interest to explore for
343 hydrothermal resources for power generation as this is the only region where the sedimentary rocks of the Cairnside
344 and Covey Hill can reach temperatures of 150 °C and more. On the other hand, in the SOM anomaly, the
345 temperature reaches 120 °C at a shallower depth, between 3,500 and 4,000 m, but in the Precambrian basement
346 because the sedimentary basin is thinner. The SOM anomaly, thus, represents a target for EGS exploration. Again,
347 the above information was inferred from the results of 3D geological modeling that is thought to better evidence
348 resource depth, magnitude and location (Figure 11).

349 The geological model was based on data from 81 oil and gas exploration wells, the surface geological map and
350 geophysical interpretations that are sparse and heterogeneously distributed both over the entire model area and at
351 depth (Bédard *et al.*, 2013). A large uncertainty with respect to temperature prediction is therefore expected for the
352 3D model where data are sparse, especially near the SOM anomaly (Figure 6). In general, the density of available
353 well data decreases toward the southeastern and deeper part of the basin.

354 Moreover, input temperature obtained from corrected BHT is the main source of uncertainty related to the evaluation
355 of temperature at depth (Bédard *et al.*, 2017). Those are not equilibrium temperature and the two anomalies
356 discussed in this manuscript are both based on one BHT data that could not be validated or invalidated and were
357 therefore included in the temperature model evidencing the present target anomalies when interpolating the surface
358 heat flow (Figure 4 and 6). Ranges of thermal conductivity and internal heat generation was previously identified for
359 each thermal unit by Bédard *et al.* (2017) based on the statistical distribution of laboratory and borehole analysis.
360 Heat flow was consequently estimated for pessimistic and optimistic scenarios, showing an average variation of

361 $\pm 35 \text{ mW m}^{-2}$, which is more than the kriging standard deviation (Figure 6). The uncertainty of the resulting
362 temperature prediction increases downward. The temperature uncertainty at 10 km depth is about 18 °C while it is
363 less than 10 °C at less than 7 km depth when considering plausible thermal property scenarios. It is important to note
364 that BHT density additionally decreases with depth. Nevertheless, this does not impact the method highlighted in this
365 contribution to assess geothermal resources of sedimentary basins with a regional 3D model. Of course, the quantity
366 of available geothermal resources can be affected by the accuracy of the temperature prediction that is subject to
367 BHT correction and thermal property uncertainties, but the location of thermal anomalies is expected to remain the
368 same regardless of in input parameter variability. This comprehensive resource assessment can be seen as a first step
369 to justify expenses to collect equilibrium temperature data in deep wells, which can be integrated to the 3D
370 temperature model to reduce its uncertainty as the stage of geothermal exploration moves one step further in the
371 SLL. For example, equilibrium temperature data have been used in the Williston basin to help correct BHT and
372 predict temperature of basal formations in 3D (Gosnold et al., 2016). In this case, the extrapolation of temperature
373 was done vertically; taking into account the thermal stratigraphy but the temperature was interpolated in 3D space
374 without building a geological model. A next step is definitely to combine equilibrium temperature data with a 3D
375 geological model to refine regional geothermal resource assessment of sedimentary basins. For the SLL basin, this
376 can be the opportunity to validate the existence of the modelled temperature anomalies.

377 The integration of steady-state conductive heat transfer equations in a 3D geological model, first achieved for the SLL
378 basin to analytically compute temperature at a regional scale and evaluate geothermal resource distribution, appears
379 to be a significant scientific development. Recent studies to estimate geothermal resources on a regional scale with
380 the same analytical heat conduction method were often based on a 2D mapping approaches (Batir *et al.*, 2016; Stutz
381 *et al.*, 2015; Palmer-Wilson *et al.*, 2018). The surface heat flow map is seen as the baseline information to estimate
382 temperature at depth with downward extrapolation assuming a uniform subsurface thermal conductivity in the crust
383 (Blackwell *et al.*, 2006; Majorowicz and Minea, 2012). The use of a 3D model allowed to compute the equivalent
384 thermal properties as function of depth, which are affected by the distribution of thermal units and the basin
385 architecture further influencing temperature and resource estimates. The surface heat flow distribution still remained
386 the baseline information in this study, but the extrapolation of temperature at depth was based on a representative
387 conceptualization of the geological units considering thermal properties changing according to unit geometry
388 (Figure 3). Additionally, simple kriging with calculation of the standard deviation was used in this study to

389 interpolate heat flow data at surface and evaluate uncertainty, which is one step further from previous assessments
390 showing interpolation results only (Blackwell *et al.*, 2006; Majorowicz and Minea, 2012; Gosnold *et al.*, 2016;
391 Palmer-Wilson *et al.*, 2018). The map of surface heat flow standard deviation allows to rapidly identify where data is
392 missing and more work should be conducted to validate or invalidate potential anomalies.

393 This estimation of geothermal resources based on a 3D geological model would not have been possible without a
394 previous assessment of thermal unit properties (Bédard *et al.*, 2017). Laboratory measurements of thermal
395 conductivity for rock samples of each unit (Nasr *et al.*, 2015; Nasr, 2016) and well log analysis to define internal heat
396 generation rates are prior information that may not be available in all regional geothermal resource assessment, but
397 essential to make appropriate use of the 3D model. Indeed, a fine regional understanding of geological setting
398 combined to a detail thermal unit characterization is needed to process with the proposed methodology. Similar work
399 has been achieved in the French Massif Central by Calcagno *et al.* (2014) and in Denmark by Fuchs *et al.* (2020), but
400 with notable differences in the methodology. These authors meshed their 3D geological model to conduct a
401 numerical simulation of steady-state heat conduction using the finite element method to determine temperature in the
402 3D space. Numerical simulations generally imply iterative computations providing approximate solutions that can be
403 meshed sensitive, has to be done with additional software from that used to build the geological model and can
404 require large computing time. On the other hand, analytical calculations done for the present work implies an exact
405 solution that is not sensitive to the shape of mesh elements and can be carried directly in the 3D geological model
406 with short computation time. However, the numerical approach provides a true 3D heat transfer simulation while the
407 analytical approach is more easily computed with 1D conductive heat transfer (vertical), but constrained from the 3D
408 geological architecture. Both methods have advantages and disadvantages that can be weighted to decide on the
409 methodology to put forward when estimating geothermal resources at the regional scale.

410 The assessment of the geothermal resources of the SLL basin was done for power generation purposes targeting host
411 rocks with temperature above 120 °C. Only a small portion of the potential resource is located in the SLL basin units
412 and is, moreover, located at more than 4 km depth where the temperature uncertainty is important. The use of such
413 low-temperature geothermal resources for power generation implies deep exploration and production drilling with
414 consequent investment. Given the depth of geothermal resources for power generation, the direct use of heat can be
415 an attractive option for future geothermal development in the context of the Province of Québec, where the
416 electricity is dominantly produced by hydroelectric power plants and is widely available at low price while space

417 heating needs remain important due to the cold climate. Further work can be done with a direct use perspective to
418 identify thermal units above 60 °C that is hot enough to be used for space heating or other applications. The
419 proximity of geothermal resources suitable for direct use with respect to population center will have to be highlighted
420 in this next step.

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425 On behalf of all authors, the corresponding author states that there is no conflict of interest.

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